APPENDIX II - Infrared Instruments (FTIRs)

Infrared spectroscopy is an analytical technique with a long history in environmental science and chemistry. For very-high-resolution spectroscopy, Fourier Transform Infrared Spectroscopy (FTIR) has supplanted other techniques because of its superior performance. This technique has been widely used in atmospheric chemistry and has been validated by exercises such as the Balloon Intercomparison Campaign (BIC) and by various validation efforts for space-based activities such as the Atmospheric Trace Molecule Spectroscopy (ATMOS) experiment, MIPAS, MOPITT, SCIAMACHY, ACE, TES, and HIRDLS. While the FTIR technique needs no further justification as a primary technique for NDACC, individual FTIR instruments, as well as other infrared instruments such as emission spectrometers, still must be validated. This description is intended to apply to the determination of vertical column amounts of trace gases, primarily by FTIR spectroscopy. High-resolution spectroscopy also can be used for deriving profiles of trace constituents, but additional validation is required for such retrievals. The NDACC Infrared Working Group (IRWG) presently is investigating the capabilities and requirements for profile retrieval; this appendix will be revised subsequently to reflect these validation requirements.

Quality Criteria for the Evaluation of New Instruments and Instrument Teams

The process of validating an infrared observing system of the NDACC is summarized in the flowchart in Figure 1. Validation is a multi-step process that may require some time to complete. Investigators proposing inclusion of their group and instrument into the NDACC / IRWG should observe the following guidelines. Further information regarding the NDACC and its Data, Measurement and Validation Protocols may be obtained at http://www.ndacc.org/ and in particular for the IRWG at http://www.acd.ucar.edu/irwg.

Minimum Requirements for Instruments and Analysis Techniques

Observing site selection is an important factor in validation. An ideal site for stratospheric observations would be at high elevation to avoid as much tropospheric water vapor as possible and away from urban centers to avoid surface-generated pollution. As the NDACC focus has broadened to tropospheric measurements, instruments at lower altitudes and closer to urban centers are acceptable. A diversity of site characteristics and global coverage are considered important, and proposals from any site would be reviewed by the IRWG. Proximity to other NDACC instruments, which employ UV, microwave, or Lidar techniques, should be established for each site. If instruments are not co-located it should be shown that the prevailing meteorology is such that measurements by the various techniques (recognized as one site) may be considered to be in the same airmass. Positioning of the sites should avoid intense local sources of the target gases.

Investigators should supply the IRWG with a detailed technical description of the site, instrument, and analysis technique. New instruments should meet the following minimum conditions:

- Maximum optical path difference: >=250 cm,
- Spectral range: 700-4100 cm-1 (minimum),
- Continuous spectral coverage (except for the 6-7 micrometer region) in a small number (less than 8) of spectral (filter) bands,
- Ability to record full-resolution spectrum (in one filter band) in approximately one minute,
- Ability to make regular timely measurements on an ongoing basis.

Not all instruments may fulfill all of these requirements but the Investigator must document their performance and the instrument will be reviewed by the IRWG. Obviously, high signal-to-noise ratio in the spectra is necessary for the detection of weak absorptions, but no specification is provided. If the proposed instrument is a commercial instrument of the same type as a previously accepted NDACC instrument, the description can be brief, referring to the accepted instrument and highlighting any differences. The IRWG (or a subcommittee thereof) will determine whether the instrument design meets NDACC requirements.

A description of the Investigator's data analysis method should be supplied, along with the sources of any supporting data such as line parameters, constituent, temperature and pressure profiles. In particular, if the technique is not currently in use in the IRWG, some comparison showing commensurate results must be offered. Ability to perform retrievals in accord with IRWG best practices and retrieval parameters must be shown.

Independent Evaluation of the Instrument Design and Data Analysis

Investigators interested in the IRWG validation process should see the following documents at the NDACC/IRWG website: IRWG_Comp-Sum_APR2009.pdf, IRWG_HBr-Cells_APR2009.pdf, IRWG_Ret-Params_APR2009.pdf, and IRWG_Val-Strat_APR2009.pdf. A sub-committee of the IRWG or referee will be designated to review the application for new instruments or investigators. The process leading to certification of a team and instrument should consist of (but is not limited to) submission to the referee of:

- Solar absorption spectra taken by the instrument at the site,
- Retrievals of several of the required NDACC gases for total columns,
- Retrievals of several of the required NDACC gases for VMR profiles,
- Spectra of a low pressure gas cell e.g. HBr with derived column and ILS data,
- Spectra and retrievals taken in a blind intercomparison if available,
- Retrievals from other spectra submitted to them and
- Error estimates of derived columns and or profiles retrieved.

Test cases should be selected which include gases with simple line structure (eg HF or HCl), complex structure (eg HNO_3) and with a known column (eg N_2 or CO_2). Species are to be selected from the list of primary archived IRWG gases. Constraints must be placed on the input temperature and pressure profiles, shape of the mixing ratio profiles

and the freedom allowed in adjusting the volume mixing ratio in the fitting for a true comparison of instrument/retrieval performance.

Through this exchange, suggestions and recommendations may be relayed to the Investigator to improve the quality of the measurements and analysis. During this time he/she is welcome at IRWG meetings to discuss their progress.

Instrument and Data Analysis Intercomparison

Before a new instrument is fully validated as part of the NDACC, a formal blind intercomparison should be performed, following the instrument intercomparison protocol. The new instrument(s) will be evaluated by comparison with one or more previously accepted NDACC instruments (reference instruments). It is highly desirable that multiple reference instruments be employed to reduce uncertainty about the origin of observed differences. It is recognized that the difficulty of moving these large delicate instruments may preclude many opportunities for multiple instrument intercomparisons; hence, these opportunities should be planned carefully by the IRWG to maximize the usefulness of the intercomparisons and to minimize cost. If one or more traveling instruments have been compared successfully with several accepted instruments, the latter can subsequently serve as transfer standards. Provisional acceptance of an instrument may be recommended by the IRWG while awaiting finalization of logistical arrangements for the formal blind intercomparison.

The intercomparison should be conducted at the NDACC site if possible. The range of solar zenith angles employed should correspond to observations at the target site(s). Observations should be made on at least five clear days. Spectra should be analyzed for no less than five of the primary NDACC molecules and N_2. Sufficient observing time should be used to ensure that random noise does not limit the retrievals substantially. Spectra should cover the entire observable spectral range. Measurements by the instrument being evaluated and the reference instrument should be as nearly coincident in time as practical. In the analysis, agreed profiles of temperature, pressure, and the constituent profile to be scaled should be used. Standard retrieval parameters currently accepted and in use by the IRWG such as spectral fitting regions, line parameters; a priori data should be used for the analysis.

After the first day of the intercomparison, quick-look data should be submitted to the referee, who may at his/her discretion, advise the participants of any major problems, thereby preventing time wasted from an unsuccessful intercomparison. Following a brief troubleshooting period based on the referee's advice, the comparison will become blind until its conclusion.

The analysis should provide the derived vertical column amount and profile for each of the target gases from the entire day's spectra and the estimated random and systematic errors in the columns and profiles. Any additional derived results, such as the instrument resolution or modulation efficiency and phase error, also should also be documented. Spectra encompassing the fitted regions used in the analysis should be

provided, along with the residuals from the fits. These results should be submitted to the referee within one month of the completion of the data collection, prior to learning the results from other instruments.

Acceptance Criteria for New Instruments

The referee or a designated subcommittee will examine the results of the intercomparison and make a recommendation to the IRWG. The recommendation will be based in part on the sensitivity of the instrument (random noise in the retrieved columns), the consistency of measurements between the evaluated and reference instruments, and the instrument performance regarding instrument line shape, zero-level errors, phase errors, and line asymmetry. The instrument / group may be accepted as a certified member of the IRWG while yet being fully validated for all retrieval species.

Quality Criteria for the Evaluation of Continuing Instruments and Teams

The Investigator has primary responsibility for ensuring the quality of data from his/her instrument on a continuing basis, and for submitting the data to the NDACC archive in a timely manner. He/she is also responsible for maintaining up-to-date documentation files describing the instrument and its quality control as outlined in the NDACC Measurement and Data Protocols.

Nevertheless, several formal tests are required periodically to ensure the data quality and intercomparability of data from different sites and to become fully validated for each species. It is impractical to bring together all of the FTIR instruments for repetitions of the instrument intercomparisons; therefore, several methods are in place for continued data quality evaluation.

For those species (e.g., ozone, water) that are measured at the NDACC site by techniques other than FTIR, continuous intercomparison of retrieved columns (and profiles, as applicable) should be performed for the purpose of maintaining confidence in both techniques as implemented at the site. IRWG members are encouraged to participate in cross instrument intercomparisons organized for this purpose. Opportunities for intercomparison with satellite measurements should be used, both for mutual evaluation and for enhancing the scientific output.

One or more mobile instruments that have been validated in intercomparison campaigns may be available for transport from site to site for side-by-side comparisons. Agreement of results from these instruments and the permanent site instruments will serve as evidence for the validity of both measuring systems. In the case of disagreement, further experiments will be needed to determine which one is not performing properly and the origin of the difficulties. For this reason, it is useful for two instruments to travel to a site for comparison with the fixed instrument. Results from all of these intercomparisons must be documented in the NDACC archive and publication

is encouraged. Because of the difficulty and cost of such comparisons, they will be relatively infrequent, perhaps every three to five years at a given site.

Each site should have one or more cells including the HBr cells constructed for this purpose, containing known amounts of gases at low pressure for routine evaluation of the instrument performance, especially the instrument line shape. The gases in question should (if possible) be linear molecules (for well-separated lines), heavy (for narrow Doppler widths), easy to handle (for convenience), and not present in detectable quantities in the atmosphere (so the cell can be used in the direct solar beam to evaluate the performance during actual data collection). This test should be performed approximately weekly, and the results included in the archive. Provision for measuring the temperature of the gas in the cell during the operation should be available.

At each meeting a subset of these cells should be brought to the site for measurement on a common instrument. The column and ILS should be determined by the hosting group and an outside IRWG member to provide a check on the analysis, instrument and the cells. Results should be archived at the IRWG web site.

If possible, monochromatic laser sources should be used to evaluate the instrument line shape. A suitable laser source perhaps could circulate with one of the traveling comparison instruments.

Investigators routinely should analyze the data for the column of gases with known concentration such as carbon dioxide (CO_2) and N_2 (and molecular oxygen, O_2, when possible); these data should be reported along with the trace gas columns. The FTIR columns should be compared regularly with the column amounts determined by other NDACC instruments at the same site where there are common species and the measurements are comparable.

There should be an ongoing exchange of spectra and analysis results among the groups. This will help prevent systematic differences in the analysis methods and provide early detection of any data quality problems, which may develop. A careful and defensible way of assessing the random and systematic errors in the retrieved columns that is consistent among the groups must be developed by the IRWG. Retrieval comparisons within the IRWG are on going and may be more or less formal. Groups are strongly encouraged to participate and take actions based on accepted improvements that result from the comparison.

It is anticipated that the processes of data collection and analysis will become more and more automated in the future. It is the Investigator's responsibility to ensure that all data archived are examined in such a way that high data quality is maintained and that undetected errors do not enter by the automation process.

Changes in Instruments and Data Analysis

Since one of the major goals of the NDACC is the detection of long-term trends, care should be used in any modifications of the instrument or data analysis, which may affect the results. Once the regular operation of an instrument has begun, such changes should not be undertaken lightly; consultation with the IRWG is recommended. The primary data (interferograms) should be retained by the investigator indefinitely so that improved data processing or retrieval techniques, including improved spectral line parameters, can be applied retrospectively to the earlier data. In such cases, the entire dataset should be reprocessed and archived, along with (at least) reference to earlier versions.

If/when an instrument is replaced an overlap of measurements should be undertaken to determine what if any artifacts from the transition may occur in the derived data products in the NDACC archive. If this is not possible for any reason, other means of certifying the new instrument as outline above may be undertaken.

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Figure 1. NDSC IRWG Path to Validation